

Magnetic field dependence of the superconducting fluctuation contribution to NMR-NQR relaxation

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Abstract

The dependence of the Maki-Thompson (MT) and of the density of states depletion (DOS) contributions from superconducting fluctuations (SF) to NMR-NQR relaxation is derived in the framework of the diagrammatic theory, applied to layered three dimensional (3D) high T_c superconductors. The regularization procedure devised for the conductivity (Buzdin and Varlamov, Phys. Rev. B, 58, 14195 (1998)) is used in order to avoid the divergence of the DOS term. The theoretical results are discussed in the light of NMR-NQR measurements in YBCO and compared with the recent theory (Eschrig *et al.*, Phys. Rev. B 59, 12095 (1999)), based on the assumption of a purely 2D spectrum of fluctuations.

75.30m, 75.40 Gb, 76.60-k, 75.25+z

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I. INTRODUCTION

The normal state of high temperature superconductors (HT_cSC) is characterized by unusual properties, most of them still lacking of a comprehensive theoretical description. In particular, the transfer of spin excitations from low to high-energy range (spin-gap opening) well above T_c , detected in the generalized susceptibility from T_1 and neutron scattering measurements (for a recent review see Ref. 1), and the related quasi-particle gap, observed in ARPES^{2,3}, have been tentatively related to superconducting fluctuations (SF) of various nature. Among them, one could mention preformed pairs without long-range phase coherence, possibly along stripes^{4,5}, spin and/or charge density waves^{6,7}, coupling of a d-wave symmetry order parameter with spin fluctuations^{8,9}, order parameter fluctuations well beyond the perturbative approach^{10–12} and quantum critical point fluctuations¹³. For a review on precursor pairing correlations and a survey of the various scenarios see Ref. 14. Furthermore the magnetic field has been argued¹⁵ to have a role on SF of overdoped HT_cSC also, by inducing a spin-gap from $T_c(0)$ to $T_c(H)$.

The role of the magnetic field is crucial in NMR-NQR attempts to study SF in the vicinity of T_c^+ . Indeed, the most direct contribution to SF, namely the Aslamazov-Larkin term, responsible of paraconductivity¹², is not effective in causing an extra-contribution to NMR-NQR relaxation. In principle, the SF contribution to the relaxation rates, for $T \rightarrow T_c^+$, are the Maki-Thompson (MT) one (related to the pairing of a carrier with itself at a previous stage of motion), and the reduction due to the depletion in the single-particle density of states (DOS), when fluctuating pairs are created¹². These two terms might have a different sensitivity to the presence of a magnetic field, which acts as a pair-breaking factor.

The first NMR experimental observation¹⁶ of the role played by SF in HT_cSC was based on the comparison of ⁶³Cu relaxation rate W in YBCO in the absence (i.e. NQR) and in the presence of a magnetic field of about 6 T. Within about 10 degrees above $T_c(0)$, $W(NQR)$ was found to decrease upon application of the field by a factor about 5÷15%. A qualitative interpretation of the experimental observation was given by assuming that the field reduced

the MT term to about 25%, while the more robust DOS term was little affected by the field. The Equations used in these estimates¹⁶ were the ones¹⁷ pertaining to a three-dimensional (3D) layered spectrum of excitations (with anisotropy parameter $r = 2\xi_c^2(0)/d^2 \simeq 0.1$, where $\xi_c(0)$ is the correlation lenght of the Cooper pair at zero temperature, along the \hat{c} -axis, and d the interlayer distance). The occurence of a pure 2D regime of SF could be ruled out, on the basis of the absolute value and of the temperature dependence of the SF contribution to ^{63}Cu .

The first systematic analysis of the field dependence of NMR relaxation rate in YBCO was carried out in 1998 by Mitrović *et al.*¹⁸, by varying the field from 2.1 up to 27.3 T. The ^{63}Cu T_1 was probed¹⁸ through the contribution to the ^{17}O echo dephasing. For field in the range 6÷8 T, the results derived in this way¹⁸ were found to coincide with the direct measurements of ^{63}Cu T_1 . At high field, W^{DOS} was argued to be strongly reduced by the field. These data¹⁸, as well as the field dependence of $^{17}\text{O}(2,3)$ Knight shift¹⁹, have been interpreted on the basis of a theory for the DOS contribution due to Eschrig *et al.*²⁰, which extended analytical approaches¹⁷ to include short wave-lenght and dynamical fluctuations, in the assumption of a 2D regime.

Recently, Gorny *et al.*²¹ reported precise ^{63}Cu relaxation measurements in YBCO for $H = 0, 8.8$ and 14.8 T, finding no magnetic field dependence in a wide temperature range. A possible dependence of the field effect on the amount of doping could be suspected since, at the same time, no field effect had been observed²² in underdoped YBCO.

In this paper we derive the magnetic field dependence of the MT and DOS contributions to NMR T_1 , in the framework of a diagrammatic description, for arbitrary values of the reduced field $\beta = 2H/H_{c2}(0)$, for a 3D layered spectrum of fluctuations, which should pertain to the case of YBCO with low anisotropy parameter. In order to remove the logarithmic divergence present in the DOS term, here we use the method devised²³ for transverse conductivity, in which regularization requirement, analogous to the ones for the nuclear relaxation rate, is present. Furthermore, we briefly discuss the role of the long wave-vector fluctuations and of the dynamical fluctuations. Our analytical conclusive expressions are compared with

the numerical solutions²⁰ for the 2D regime and with the experimental measurements carried out until now.

II. FIELD DEPENDENCE OF THE SF CONTRIBUTION NUCLEAR RELAXATION

In the following, we extend the diagrammatic theory for the SF contribution to NMR-NQR relaxation rate, to include the effects due to the presence of a magnetic field along the \hat{c} -axis, in HT_cSC.

In the presence of the field the MT and DOS contributions to the relaxation rates^{12,17} must be evaluated by starting from the usual inclusion in the momentum \mathbf{q} of the term $(-2e/c)\mathbf{A}$, with $\mathbf{A} = \frac{B}{2}(-y\mathbf{i} + x\mathbf{j})$. The integration over \mathbf{q} , in the ab plane, is substituted by a sum over the Landau levels. Thus the MT and DOS contributions¹⁷ to W assume the forms

$$\frac{W^{MT}}{W^0}(\beta, \varepsilon) = \frac{\pi}{8E_F\tau} \frac{\beta}{(\varepsilon - \gamma_\varphi)} \cdot \sum_n \left[\frac{1}{\sqrt{\gamma_\varphi + \beta(n + 1/2)}} \frac{1}{\sqrt{\gamma_\varphi + \beta(n + 1/2) + r}} + \right. \\ \left. - \frac{1}{\sqrt{\varepsilon + \beta(n + 1/2)}} \frac{1}{\sqrt{\varepsilon + \beta(n + 1/2) + r}} \right] \quad (1)$$

and

$$\frac{W^{DOS}}{W^0}(\beta, \epsilon) = -\frac{\hbar}{E_F\tau} \cdot \kappa(T\tau) \cdot \sum_n^{1/\beta} \frac{1}{\sqrt{\varepsilon + \beta(n + 1/2)}} \frac{1}{\sqrt{\varepsilon + \beta(n + 1/2) + r}} \quad (2)$$

where W^0 is the ordinary relaxation rate in the absence of SF (the Korringa one in a Fermi gas-like model). In the above Equations, E_F is the Fermi energy, τ the single particle collision time, $\gamma_\varphi = \xi_0^2/\mathbf{D}\tau_\varphi$ (with $\mathbf{D} = E_F\tau/m$, 2D carrier diffusion constant and $\hbar\tau_\varphi^{-1}$ depairing energy) is a dimensionless factor which, in the limit $B \rightarrow 0$, takes into account the pair-breaking effect and $\varepsilon = (T - T_c)/T_c$ is the reduced temperature. $\kappa(T\tau)$ in Eq. (2) is the function

$$\kappa(T\tau) = \frac{7\zeta(3)}{\pi} \frac{1}{4\pi T\tau [\psi(1/2) - \psi(1/2 + 1/4\pi T\tau)] + \psi'(1/2)} = \begin{cases} \frac{14\zeta(3)}{\pi^3}, & T\tau \ll 1 \\ 4T\tau, & T\tau \gg 1 \end{cases}$$

where, $K_B = \hbar = 1$ and ψ is the Euler digamma function. The expressions (1) and (2) are general and hold for any magnetic field, provided that $\beta = 2B/B_{c2}(0) \ll 1$ (see Ref. 24).

The DOS term shows a logarithmic divergence in the sum.

The behaviours of W^{MT} and W^{DOS} , for small fields, can easily be derived from Eqs. (1) and (2), by a straightforward expansion. The intermediate and strong field regimes, namely $\varepsilon \ll \beta \ll 1$, require some care. For the MT contribution (Eq. (1)) the sum over n converges rapidly and thus, for strong fields, only the term $n = 0$ can be taken into account. For the DOS contribution (Eq. (2)), however, the logarithmic divergence must be removed. This can be achieved by considering the cut-off independent difference

$$\Delta W^{DOS}(\beta, \varepsilon) \equiv W^{DOS}(\beta, \varepsilon) - W^{DOS}(0, \varepsilon) \quad (3)$$

The zero field expression is rewritten in the form

$$\frac{W^{DOS}(0, \varepsilon)}{W^0} = -\frac{\hbar}{E_F \tau} \cdot 2\kappa(T\tau) \lim_{\beta \rightarrow 0} \sum_{n=0}^{1/\beta} \ln \frac{\sqrt{\varepsilon + \beta n + \beta} + \sqrt{\varepsilon + r + \beta n + \beta}}{\sqrt{\varepsilon + \beta n} + \sqrt{\varepsilon + r + \beta n}} \quad (4)$$

and then, Eq. (3) becomes

$$\begin{aligned} \frac{\Delta W^{DOS}(\beta, \varepsilon)}{W^0} &= \frac{\hbar}{E_F \tau} \cdot 2\kappa(T\tau) \sum_{n=0}^{\infty} \left\{ \ln \frac{\sqrt{\varepsilon + \beta n + \beta} + \sqrt{\varepsilon + r + \beta n + \beta}}{\sqrt{\varepsilon + \beta n} + \sqrt{\varepsilon + r + \beta n}} + \right. \\ &\quad \left. - \frac{\beta}{2\sqrt{\varepsilon + \beta n + \beta/2}\sqrt{\varepsilon + r + \beta n + \beta/2}} \right\} \end{aligned} \quad (5)$$

where the summation has been extended up to $n \rightarrow \infty$, since $\Delta W^{DOS}(\beta, \varepsilon)$ now involves a summation which is convergent (the n -th term being proportional to $n^{-3/2}$ for large n).

Now we are going to discuss the behaviours of W^{DOS} and W^{MT} in the asymptotic limits, corresponding to different temperature and field regimes.

A. Weak magnetic fields

In the weak field regime, namely $\beta \ll \varepsilon$, Eqs. (1), (2) can be expanded in powers of β . For the DOS term, in particular, the Euler-MacLaurin formula

$$\sum_{n=0}^N f(n) = \int_0^N f(x)dx + \frac{1}{2}[f(N) + f(0)] + \frac{1}{12}[f'(N) - f'(0)] + \dots$$

yields

$$\frac{W^{MT}}{W^0}(\beta \ll \varepsilon) = \frac{\pi}{8E_F\tau} \frac{1}{\varepsilon - \gamma_\varphi} \left[2 \ln \left(\frac{\varepsilon^{1/2} + (\varepsilon + r)^{1/2}}{\gamma_\varphi^{1/2} + (\gamma_\varphi + r)^{1/2}} \right) + \right. \\ \left. - \frac{\beta^2}{24} \left(\frac{\gamma_\varphi + r/2}{[\gamma_\varphi(\gamma_\varphi + r)]^{3/2}} - \frac{\varepsilon + r/2}{[\varepsilon(\varepsilon + r)]^{3/2}} \right) \right] \quad (6)$$

$$\frac{W^{DOS}}{W^0}(\beta \ll \varepsilon) = -\frac{\hbar}{E_F\tau} \cdot \kappa(T\tau) \left[2 \ln \left(\frac{2}{\varepsilon^{1/2} + (\varepsilon + r)^{1/2}} \right) + \right. \\ \left. - \frac{\beta^2(\varepsilon + r/2)}{24[\varepsilon(\varepsilon + r)]^{3/2}} \right] \quad (7)$$

B. Intermediate and strong field regimes

For the MT term in the strong field regime ($\beta \gg \max\{\varepsilon, r, \gamma_\varphi\}$), by expanding Eq. (1) in powers of β^{-1} , one has

$$\frac{W^{MT}}{W^0}(\varepsilon, \gamma_\varphi, r \ll \beta) = \frac{3\pi^3}{16E_F\tau} \frac{1}{\beta} \quad (8)$$

In the intermediate case (namely $\varepsilon, \gamma_\varphi \ll \beta \ll r$ and $\varepsilon \ll \beta \ll \gamma_\varphi, r$), which can become relevant for a 3D layered compound, the series expansions in terms of the smallest parameters yield

$$\frac{W^{MT}}{W^0}(\varepsilon, \gamma_\varphi, \ll \beta \ll r) = 4.57 \frac{\pi}{16E_F\tau} \frac{1}{\sqrt{\beta r}} \quad (9)$$

$$\frac{W^{MT}}{W^0}(\varepsilon \ll \beta \ll \gamma_\varphi, r) = \frac{\pi}{8E_F\tau} \frac{1}{\gamma_\varphi} \ln \frac{\sqrt{\max\{\gamma_\varphi, r\}}}{\sqrt{\beta} + \sqrt{\beta + r}}. \quad (10)$$

For the field dependence of the DOS correction to the zero field contribution (Eq. (5)), in strong field regime, one can take into account the $n = 0$ term only:

$$\frac{\Delta W^{DOS}(\beta \gg \max\{\varepsilon, r\})}{W^0} = \frac{\hbar}{E_F\tau} \cdot 2\kappa(T\tau) \left\{ \ln \frac{2\sqrt{\beta}}{e(\sqrt{\varepsilon} + \sqrt{\varepsilon + r})} \right\} \quad (11)$$

The $n \geq 1$ terms, neglected in this evaluation, yield a correction of 0.02 in the bracket term in Eq (11).

In the intermediate fields, namely for $\varepsilon \ll \beta \ll r$ (corresponding to a 3D layered regime of fluctuations), by means of an expansion of Eq. (5) in terms of $\beta/2r$ one has

$$\frac{\Delta W^{DOS}(\varepsilon \ll \beta \ll r)}{W^0} = 0.428 \frac{\hbar}{E_F \tau} \cdot \kappa(T\tau) \sqrt{\frac{\beta}{2r}}. \quad (12)$$

III. DISCUSSION AND COMPARISON WITH EXPERIMENTAL RESULTS

As it appears from the theoretical treatment given in the previous Section, the dependence on the magnetic field of the SF contributions to the NMR-NQR relaxation rate is a rather delicate issue, because of the non-trivial interplay of several parameters, such as $(T - T_c)$, the reduced field $\beta = 2B/B_{c2}(0)$, the anisotropy parameter r , the elastic collision time τ and the anelastic phase-breaking time τ_φ .

Eschrig *et al.*²⁰, in their numerical extension of the previous analytical approaches¹⁷, have considered arbitrary values of $\kappa(T\tau)$ and taken into account short wave-length and dynamical fluctuations. However, this generalization has required the restriction to a purely 2D regime of SF, which seems questionable in view of experimental findings in YBCO, pointing out a crossover to 3D fluctuations well above T_c , at least for relatively small fields^{25–27}. On the other hand, it could be remarked that dynamical fluctuations are relevant only when the field is comparable to $B_{c2}(0) \sim 100 \div 120$ T. Therefore the reduction to static and small wave-vector fluctuations should not invalidate our conclusive expressions given above.

To illustrate the theoretical expressions, derived in Section II, we plot in Figs. 1 and 2 the temperature and field behaviours of W^{DOS} and W^{MT} , with a choice of parameters appropriate to YBCO optimally doped.

In Fig. 3 the experimental results from various authors (and from different YBCO samples, about optimally doped) are compared with the behaviour expected for DOS contribution, according to Eqs. (3) and (5). A relatively small field dependence, of both DOS and MT contributions, up to a reduced field of about 0.2, is noticed. For strong fields a reduction of the MT term can be expected, while the DOS term seems only slightly affected

(see Figs. 1b and 2b). As a consequence, either for s-symmetry of the fluctuating Cooper pair (namely, presence of both the MT and DOS effects of SF on T_1) or for d-symmetry (and therefore, no MT contribution) only a slight dependence of T_1 , on the magnetic field, should be detected, as it is illustrated in Fig. 3, for the DOS term. In particular the experimental data¹⁸ at strong fields ($\beta > 0.2$) can hardly be justified. The discrepancy between the theoretical description and the experimental findings, at strong fields, might be related to the general framework involved in our treatment. However, it should be stressed that a breakdown of the Fermi liquid picture should not invalidate the expression for the DOS contribution, which is independent from the pairing mechanism and the normal state properties. The dimensional crossover (3D→2D) for strong fields is taken into account in our equations, but it could be argued that dynamical and short wave-length fluctuations are no longer negligible in a 2D strong field regime. Finally, it should be taken into consideration the possibility that the method of an indirect estimate of ^{63}Cu T_1 from ^{17}O echo dephasing¹⁸ could be invalidated in strong fields.

Summarizing, from the behaviour of ^{63}Cu $T_1^{16,18,19,21}$ one can infer that a DOS SF contribution to the nuclear relaxation is present in the vicinity of T_c . The MT term is more elusive, requiring a s-wave component in the spectrum of the SF and being possibly strongly sample-dependent, through the pair-breaking and impurities effects. The field dependence of DOS term is a rather delicate issue, complicated by various crossovers and parameters. Further theoretical and experimental work is required for a firm conclusion.

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CAPTIONS FOR FIGURES

Fig. 1: Theoretical behaviours for the DOS contribution to the nuclear spin-lattice relaxation rate (normalized to the value in the absence of SF, W^0), according to Eqs. (3) and (5), in the text, as a function of temperature for different values of the field (a), and as a function of the reduced magnetic field $\beta = 2B/B_{c2}(0)$ for fixed values of the temperature (b). The curves have been derived in correspondence to choices of the upper critical field $B_{c2}(0) \sim 120$ T, the Fermi energy $E_F = 3500$ K_B and the single-particle collision time $\tau = 2 \cdot 10^{-14}$ s.

Fig. 2: Theoretical behaviours for the MT contribution to the nuclear spin-lattice relaxation rate, according to Eq. (1), in the case of strong pair-breaking ($\gamma_\varphi \simeq 0.3$). Part (a) of Fig. 2 shows $W^{MT}(\beta, \varepsilon)/W^0$ as a function of temperature (for different values of the field) while part (b) reports it as a function of the reduced field, $\beta = 2B/B_{c2}(0)$, in correspondence to fixed values of the temperature. The choice of parameters is the same as in Fig. 1.

Fig. 3: Comparison between the experimental results, obtained at $T \simeq 95$ K (\square Mitrović *et al.*¹⁸; \diamond Gorny *et al.*²¹; \square da Carretta *et al.*¹⁶; \times da Carretta *et al.* (data unpublished)) and the theoretical predictions for the DOS term as a function of the reduced field in correspondence to the usual choice of parameters (Figs. 1 and 2). The experimental data by Gorny *et al.*²² (\diamond) and by Carretta *et al.* (\times) (unpublished) have been reported in correspondence to the value $W^{DOS}(0, \varepsilon) \simeq -0.16W^0$, in order to analyze their possible field dependence.





